

Model of a hypothetical high-temperature superconductor.

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We propose a model of a hypothetical superconductor which includes impurities with retarded interaction with quasiparticle and superconducting matrix where these impurity can be applied with large concentration. Interaction between the impurity and a conduction electron in such a system has been calculated. We have found the critical temperature of the system matrix+impurity essentially exceeds critical temperature of the pure superconducting matrix.

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I. INTRODUCTION

As it is well known at embedding of impurities in a superconductor a gap Δ and an energetic parameter ε are renormalized [1, 2]. If the superconductor is s-wave type and impurities are nonmagnetic then the gap and the energetic parameter ε are renormalized equally: $\frac{\tilde{\Delta}}{\tilde{\varepsilon}} = \frac{\Delta}{\varepsilon}$, where $\tilde{\Delta}, \tilde{\varepsilon}$ are renormalized values by an impurity scattering. As a consequence a critical temperature of a superconductor does not change. This statement is Anderson's theorem. If d-wave pairing takes place or impurities are magnetic or electrons are paired with nonretarded interaction (as in BCS theory [3]) then the gap and the energetic parameter are renormalized in different ways: $\frac{\tilde{\Delta}}{\tilde{\varepsilon}} < \frac{\Delta}{\varepsilon}$. Hence the critical temperature decreases and an effect of gapless superconductivity can take place. In a work [4] generalization of a disordered metal's theory has been proposed when scattering of quasiparticles by nonmagnetic impurities is caused with a retarded interaction. The retarded interaction occurs because the impurities have an internal structure and make transitions between their states under the action of metal's quasiparticles. It was shown that in this case embedding of the impurities in s-wave superconductor increases its critical temperature. The increase of the critical temperature is a mathematical consequence of an inequality $\frac{\tilde{\Delta}}{\tilde{\varepsilon}} > \frac{\Delta}{\varepsilon}$, that is the gap and the energetic parameter are renormalized in the opposite way to a case of magnetic impurities. It should be notice that the disorder can influence upon phonon and electron specter in materials. Experiments in superconductive metal showed suppression of T_C by a sufficiently strong disorder [6–9]. The strong disorder means that a free length l is such that $\frac{1}{k_F l} \approx 1$ or $\varepsilon_F \tau \approx 1$, where $\tau = l/v_F$ is a mean free time. Collapse of superconducting state takes place near Anderson's transition metal-insulator, that is when $\frac{1}{k_F l} \gtrsim 1$. In a work [5] a perturbation theory and a diagram technique have been developed for a disordered metal if interaction of quasiparticles with impurities is retarded and impurity's oscillations are local. Transition amplitudes of the impurities between their states under the action of metal's quasiparticles (an electron-impurity coupling) have been obtained in the adiabatic approximation. Eliashberg equations at a critical temperature T_C^* have been generalized for a case of s-wave superconductor containing impurities of a considered type. It found a critical temperature of a system metal+impurity is more than a critical temperature of the pure metal $T_C^* > T_C$. In the works [4, 5] it has been shown that the equations for the transition temperature T_C^* of the system metal+impurity can be simplified if we calculate so-called singularity temperature T^* only. The singularity temperature is a superconducting transition temperature if we turn off the pairing interaction caused by metal's phonon, therefore we have always $T^* < T_C^*$. The singularity temperature can be used as a lower estimate of the critical temperature of the dirty metal if $T^* \gg T_C$.

In the articles [4, 5] principal possibility of increasing of the superconductive transitional temperature has been shown and method of calculation of the transition temperature was given. However in these articles a model of an impurity was not proposed. Hence this paper is aimed to propose the model of the impurity with retarded interaction with quasiparticle, to propose superconducting matrix where these impurities can be applied, to calculate the singularity temperature and critical temperature for the system matrix+impurity.

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II. MODEL OF AN IMPURITY.

A. Structure of the impurity.

The impurity must have internal structure that is to have possibility to be in states with different energies. The simplest example of this system is a harmonic oscillator. Moreover metal's quasiparticles must interact with the impurities. We offer the following construction of the impurity. Large variety of endohedral complexes - atoms and ions inside the C_{60} cage is known now [10]. For our aim endohedral complexes $X@C_{60}$, where X is a noble gas atom (He , Ne , Ar , Kr , Xe) trapped in a carbon cage [11–15], are suitable. Since the noble gas atom has closed electron shell then it does not transfer charge to the cage and it is in central of the cage (thereby no breaking the symmetry of the fullerene) unlike metal endohedral complexes where an atom of metal is shifted to internal surface of the cage. Moreover the central noble gas atom does not change chemical properties of a fullerene unlike atom of metal.

Noble gas atom interacts with carbon cage by van der Waals interaction. As it was explained in [10, 16, 17] on an example of a complex $N@C_{60}$ (nitrogen like a noble gas atom does not make a covalent bond with a carbon cage, however it has nonzero spin) a fullerene has inner cavity in its center - Fig.1. Size of the inner cavity is $\Delta R = R(C_{60}) - R_W(C) = 1.87\text{\AA}$, where $R(C_{60}) = 3.57\text{\AA}$ is a radius of fullerene, $R_W(C) = 1.70\text{\AA}$ is van der Waals radius of a carbon atom. An atom X can be placed into the inner cavity if $R_W(X) \lesssim \Delta R$. Van der Waals radii of noble gas atoms are $R_W(He) = 1.40\text{\AA}$, $R_W(Ne) = 1.54\text{\AA}$, $R_W(Ar) = 1.88\text{\AA}$, $R_W(Kr) = 2.02\text{\AA}$, $R_W(Xe) = 2.16\text{\AA}$. Thus He , Ne , Ar can be placed into fullerene [11]. If $R_W(X) \gtrsim \Delta R$ then van der Waals attraction acts between noble gas atom and the carbon cage. Therefore when we place atoms He , Ne , Ar in the cage we have an energy gain, and when we place atoms Kr , Xe in the cage we increase energy of the system [18].

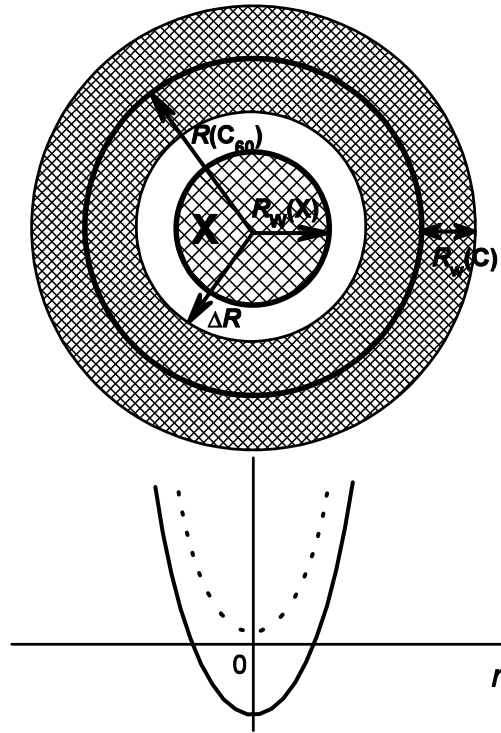


Рис. 1: Cross-section of an endohedral fullerene $X@C_{60}$. We consider the carbon cage as a spherical layer of thickness $2R_W(C)$ and central radius $R(C_{60})$. An atom X is a central noble gas atom of van der Waals radius $R_W(X)$ placed into the inner cavity of radius ΔR . In lower part of the figure the potential energy of the noble gas atom in C_{60} is shown schematically as a function of displacement from the center. For He , Ne , Ar the energy are shown by a solid line. We can see an energy gain. For Kr , Xe the energy are shown by a dotted line. We can see positive energy of the atoms in the fullerene.

The simplest endohedral fullerene is $He@C_{60}$. In a work [19] a potential energy of $He@C_{60}$ relative to noninteracting He and C_{60} as a function of the He displacement from the center of C_{60} has been calculated with density functional

method assuming no relaxation of the cage atoms. For two model potentials they obtained:

$$V_1(r) = (0.8098r^6 + 0.8428r^4 + 1.905r^2 - 2.001)\text{kcal/mol} \quad (1)$$

$$V_2(r) = (0.6706r^6 + 0.5367r^4 + 1.370r^2 - 1.999)\text{kcal/mol}, \quad (2)$$

where r is a displacement of a helium atom from the center of C_{60} (in angstroms). Thus the energy gain for He inside C_{60} is 1000K (we will use a system of units where $\hbar = k_{\text{B}} = 1$). If the potential (1,2) are consider as harmonic, then corresponding frequencies and corresponding oscillator lengths are

$$\omega_1 = 151\text{K}, \quad \xi_1 = 0.28\text{\AA} \quad (3)$$

$$\omega_2 = 128\text{K}, \quad \xi_2 = 0.31\text{\AA}. \quad (4)$$

The oscillator lengths are average displacements of a helium atom from the center of C_{60} . Since $\xi_{1,2}^2 \gg \xi_{1,2}^4 \gg \xi_{1,2}^6$ then we can keep the quadratic terms in Eqs.(1,2) only. The potential energy can be measured from the bottom of the potential well: $V_{1,2}(0) = 0$. This means harmonic approximation for potential energy of a helium atom in a center of fullerene. Then energy of the atom in a center of a fullerene is energy of a 3D harmonic oscillator

$$E = \omega \left(2n + l + \frac{3}{2} \right), \quad (5)$$

where n is a main quantum number, l is an orbital quantum number, and besides a magnetic quantum number is $m = -l, -l+1, \dots, l-1, l$. States of the noble gas atom in a center of a fullerene are states of a 3D harmonic oscillator: $\Psi_{n,l,m}(r, \theta, \varphi) = R_{n,l}(r)Y_{l,m}(\theta, \varphi)$, where $R_{n,l}(r)$ is a radial function, $Y_{l,m}(\theta, \varphi)$ is an orbital wave function.

B. Interaction with electrons.

Let the endohedral fullerene He@C_{60} is embeded into into electron gas in a conductor. The most suitable system for our aim is an alkali-doped fulleride, for example K_3C_{60} . In alkali-doped fullerides the molecules C_{60} are not impurities but they is placed regularly in a crystal lattice. A lattice constant is $a = 14.23\text{\AA}$. There are 4 molecules of fullerene per a lattice cell. In each fullerene we can placed helium atom, then we have a substance $\text{K}_3\text{He@C}_{60}$ - Fig.(2), where the helium atoms can be considered as impurities (justification is in Section III). Electrons interacts with a carbon cage and with a central helium atom of the endohedral fullerene. The carbon cage is made with σ -bonds of $1s$ electrons of carbon atoms (very small overlap), σ -bonds of $2sp^2$ hybridized electrons and π -bonds of 60 $2p$ electrons distributed over 8 Huckel orbits due truncated icosahedron symmetry of a fullerene. In the molecule there are the highest occupied molecular orbital (HOMO) h_{1u} occupied by 10 electrons with energy $\approx -5.8\text{eV}$ and the lowest unoccupied molecular orbital (LUMO) t_{1u} which can carry 6 electrons with energy $\approx -4.2\text{eV}$ [20]. An overlap of empty t_{1u} levels of neighbour fullerenes forms a conduction band of width $\approx 0.5\text{eV}$ [22–24]. Each alkali metal atom give one electron so that each fullerene obtains three electron, that is t_{1u} level is filled to half. Accordingly the conduction band is filled to half too and the alkali doped fulleride is a conductor [25].

Let us consider intramolecular interaction of an excess electron on t_{1u} level (a conduction electron) with oscillations of the endohedral fullerene He@C_{60} . To describe the interaction we use *orthogonalized plane wave method* and *pseudopotential method* [21]. This method is applied for description of a conduction electron in a metal, where state of the electron is a plane wave $\frac{1}{V}e^{i\mathbf{k}\mathbf{r}}$ between ions and *rapidly oscillating function* $\psi_{n,l,m}(\mathbf{r})$ (wave function of a valent atomic orbital) near each ion. *The oscillations increase kinetic energy of an electron near an ion. The increasing of kinetic energy acts in the vicinity of the ion cores like some repulsive potential.* Huckel orbits of an endohedral fullerene He@C_{60} is formed from overlap of orbits of a carbon cage (σ -bonds and π -bonds) and $1s$ -state of a helium atom. As a result we have new orbits, but, in consequence of the small overlap of orbits of C_{60} and He , energy of electron's states is changed little. However fact of the overlap influences on states of conduction electrons as follows. The conduction band is formed of overlap of the valent t_{1u} states of neighboring molecules. As for atoms in the orthogonalized plane wave method, the wave function φ of a conduction electron with energy E are orthogonal to the occupied states, in particular to $1s$ -state of an electron in the helium atom χ :

$$\langle \varphi | \chi \rangle = 0, \quad \chi = \frac{1}{\sqrt{\pi a^3}} e^{-r/a} \quad (6)$$

where $a = 0.31\text{\AA}$ is atomic radius, $E_\chi = -38.83\text{eV}$ is energy of the electron in $1s$ -state. The orthogonality takes into consideration above-mentioned rapid oscillations of the conduction electron's wave function near the molecular core. The rapid oscillations give an additional kinetic energy $\sim \int_0^a \varphi^+ \Delta \varphi d\mathbf{r}$ in vicinity of the molecular cores. The

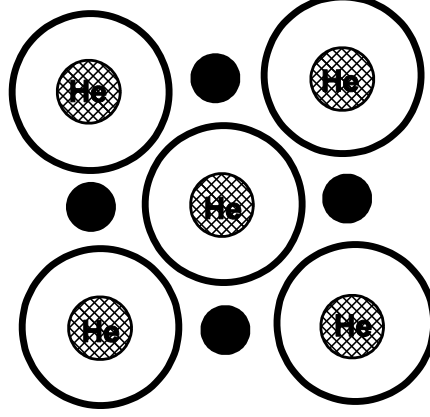


Рис. 2: Plane (100) face-centered cubic lattice of $K_3\text{He}@C_{60}$. Big circles are fullerene molecules, small black circles are alkali ions, circles in center of the fullerene are helium atoms.

pseudopotential method allows us to rewrite the kinetic energy as some effective potential U_{eff} - pseudopotential, and unknown exact wave function of a valent electron can be replaced by some pseudowave function ψ which has not rapid oscillations near a molecular (ionic) core, but this state has energy which is the same as in the exact state - E . Then according to [21] the effective potential can have a form

$$\hat{U}_{\text{eff}} = \hat{U} + (E - E_\chi) |\chi\rangle\langle\chi| \equiv \hat{U} + \hat{U}_{\text{ps}}. \quad (7)$$

The second part of the potential is repulsive because energy of a valent electron E is more then energy of ionic core $E > E_\chi$. The repulsive pseudopotential is manifestation of the Pauli principle prohibiting the valence electrons to be in region of the occupied orbitals (in our case in region of the occupied 1s-orbital of a helium atom). Mathematically this fact is expressed by the orthogonality (6).

In coordinate representations the effect on a wave function and an quantum-mechanical average of the pseudopotential are correspondingly:

$$\hat{U}_{\text{ps}}|\psi\rangle = (E - E_\chi) \chi(\mathbf{r}) \int \chi(\mathbf{r}')\psi(\mathbf{r}')d\mathbf{r}' \quad (8)$$

$$\langle\psi|\hat{U}_{\text{ps}}|\psi\rangle = (E - E_\chi) \int \chi(\mathbf{r})\psi(\mathbf{r})d\mathbf{r} \int \chi(\mathbf{r}')\psi(\mathbf{r}')d\mathbf{r}' \quad (9)$$

We can see the pseudopotential is a nonlocal operator. The function $\chi(\mathbf{r})$ plays a role of a formfactor. Using of the nonlocal operator is problematical. However the nonlocal pseudopotential can be localized taking into account the effects of nonlocality. We propose a following method. Let us write the localized pseudopotential in a form (we take out the function ψ under the integral sign in Eq.(8)):

$$\hat{U}_{\text{loc}} = A (E - E_\chi) \chi(\mathbf{r}) \int \chi(\mathbf{r}')d\mathbf{r}' = 8A (E - E_\chi) e^{-\frac{r}{a}}, \quad (10)$$

where a constant A is found from equality of quantum-mechanical averages:

$$\langle\psi|\hat{U}_{\text{ps}}|\psi\rangle = \langle\psi|\hat{U}_{\text{loc}}|\psi\rangle. \quad (11)$$

Thus constant A considers nonlocality of the pseudopotential. In the first approximation the pseudowave function can be chosen as a plane wave $\psi = \frac{1}{\sqrt{V}}e^{i\mathbf{k}\mathbf{r}} \equiv |\mathbf{k}\rangle$. Then we have

$$\langle\mathbf{k}|\hat{U}_{\text{ps}}|\mathbf{k}\rangle = \frac{64\pi}{V} (E - E_\chi) a^3 A \quad (12)$$

$$\langle\mathbf{k}|\hat{U}_{\text{loc}}|\mathbf{k}\rangle = \frac{64\pi}{V} (E - E_\chi) a^3 (1 + a^2 k^2)^{-4}. \quad (13)$$

Hence $A = (1 + a^2 k^2)^{-4}$, where we can suppose $k = k_F$. As one would expect the nonlocality somewhat weakens the interaction. The localized pseudopotential in coordinate space and in momentum spaces is

$$\hat{U}_{\text{loc}}(r) = \frac{8(E - E_\chi)}{(1 + a^2 k_F^2)^4} e^{-\frac{r}{a}} \quad (14)$$

$$\hat{U}_{\text{loc}}(q) = \int e^{-i\mathbf{kr}} \hat{U}_{\text{loc}}(r) d\mathbf{r} = \frac{64\pi(E - E_\chi)}{(1 + a^2 k_F^2)^4} \frac{a^3}{(1 + a^2 q^2)^2}. \quad (15)$$

Let us consider the potential U in Eq.(7). In the pseudopotential method for a metal the potential is Coulomb $-\frac{e^2 Z}{r}$, where $Z \neq 0$ is a degree of ionization of an atom. Then contribution of the first term in Eq.(7) is negative, contribution of the pseudopotential is positive. Thus compensation of these two terms takes place. This leads to a weak resulting potential U_{eff} [21]. In our case a helium atom in an endohedral fullerene is neutral $Z = 0$. Thus the compensation does not take place and the pseudopotential is a strong repulsive potential unlike a metal. Interaction of an electron with an atom is

$$U(q) = -\frac{4\pi e^2}{q^2} (Q - n_{\mathbf{q}}) = -\frac{2e^2}{q^2} \left(1 - \left(1 + \frac{a^2}{8} q^2 \right)^{-2} \right), \quad (16)$$

where Q is a nuclear charge and $n_{\mathbf{q}}$ is Fourier transform of electron density [26]. The potential for a neutral helium atom is weak short range. Estimation of values of the pseudopotential (15) and the potential (16) shows $U_{\text{loc}} \gg U$, so that the potential U can be omitted and $U_{\text{eff}} = U_{\text{loc}}$.

III. SUPERCONDUCTIVITY

A. General equations

Conduction electrons interact with intramolecular $\text{Hg}(1) - \text{Hg}(8)$ phonons which have frequencies $273 - 1575 \text{ cm}^{-1}$ [25]. The interaction results to superconductivity of alkali-doped fullerenes. So, in a substance K_3C_{60} a critical temperature is $T_C = 19.3\text{K}$. In this section we consider an influence of interaction with a helium atom in an endohedral fullerene He@C_{60} on superconducting properties of alkali doped fulleride. In other words our aim is to find the critical temperature of a substance $\text{K}_3\text{He@C}_{60}$.

Let an electron moves in a field created by N scatterers (impurities) which are placed in points \mathbf{R}_j by a random manner with concentration $\rho = \frac{N}{V}$. Such system is spatially inhomogeneous, hence momentum of a quasiparticle is not conserved. However we can use mean-field approximation, that is effect of all impurities is replaced by a mean field using an averaging operation over a disorder. The operation for a propagator of a quasiparticle has a form [27]:

$$\langle G(x, x') \rangle = -i \left\langle \frac{\langle \hat{T} \psi^+(x) \psi(x') \hat{U} \rangle_0}{\langle \hat{U} \rangle_0} \right\rangle_{\text{disorder}}, \quad (17)$$

where \hat{U} is an evolution operator, $\langle \dots \rangle_0$ is done over a ground state of Fermi system and a lattice (in the numerator and the denominator separately). The averaging over the disorder is done in the following way - at first the propagator is calculated at the given disorder, and only then the averaging $\langle \dots \rangle$ is done (the whole fraction is averaged). The averaging over an ensemble of samples with all possible positions of impurities recovers spatial homogeneity of the system, hence quasiparticles' momentums are conserved. Practically the averaging $\langle \dots \rangle_{\text{disorder}}$ is done as follows:

$$\sum_j \mathbf{R}_j \longrightarrow \rho \int d\mathbf{R}, \quad (18)$$

where ρ is concentration of impurities. Thus the impurities are "smeared" over the system with concentration ρ and they act on quasiparticles as a mean field. Diagram technique for disordered system if interaction of quasiparticles with impurities is retarded has been developed in a work [5].

On the other hand we propose a substance $\text{K}_3\text{He@C}_{60}$, where the molecules He@C_{60} is not impurities but they are placed regularly in a crystal lattice - Fig(2). This system can be considered in an approximation of a jelly model. In

this model the helium atoms are "smeared" over the system like electron and ion subsystems in a metal and they act on quasiparticles as a mean field. Thus the jelly model leads to the same result as the averaging (17) in the disordered metal with concentration of impurities $\rho = 4/a^3$, where $a = 14.23\text{\AA}$ is a lattice constant and 4 molecules of fullerene per a lattice cell are. However there is a significant difference of these model. As it is well known impurities in a metal result to decreasing of density of states at Fermi surface up to Anderson localization if density of the impurities is large [1, 2]. The decreasing is result of scattering of conduction electrons by randomly distributed impurities. In $\text{K}_3\text{He}@\text{C}_{60}$ we have a regular arrangement of helium atoms that does not result to decreasing of the density of states on Fermi surface and Anderson localization.

Let us calculate critical temperature T_{C}^* of a system $\text{K}_3\text{He}@\text{C}_{60}$, where helium atoms play a role of an impurity. Critical temperature of a pure system K_3C_{60} is $T_{\text{C}} = 19.3\text{K}$. In a work [5] Eliashberg equations has been generalized for a system metal+impurities. The impurity is a harmonic oscillator with transition frequencies between any of its states ϕ_B and ϕ_A : $\omega_{AB} = E(B) - E(A)$, interaction of a conduction electron with the impurity is $U(r)$, the impurities are distributed over the system with concentration ρ . The conduction electrons interact with phonon with frequency ω_{D} , electron-phonon coupling constant is g . The equations have a form

$$Z(\varepsilon_n)\Delta_n = \sum_{m=-\infty}^{+\infty} (L(n-m) - \mu^*) \frac{\pi T \tilde{\Delta}_m}{\sqrt{\tilde{\varepsilon}_m^2 + |\tilde{\Delta}_m|^2}} \quad (19)$$

$$(1 - Z(\varepsilon_n))\varepsilon_n = \sum_{m=-\infty}^{+\infty} L(n-m) \frac{\pi T \tilde{\varepsilon}_m}{\sqrt{\tilde{\varepsilon}_m^2 + |\tilde{\Delta}_m|^2}}, \quad (20)$$

$$\tilde{\Delta}_n = \Delta_n + \sum_{m=-\infty}^{+\infty} W(n-m) \frac{\pi T \tilde{\Delta}_m}{\sqrt{\tilde{\varepsilon}_m^2 + |\tilde{\Delta}_m|^2}} \quad (21)$$

$$\tilde{\varepsilon}_n = \varepsilon_n + \sum_{m=-\infty}^{+\infty} W(n-m) \frac{\pi T \tilde{\varepsilon}_m}{\sqrt{\tilde{\varepsilon}_m^2 + |\tilde{\Delta}_m|^2}}, \quad (22)$$

where $\varepsilon_n = \pi T(2n+1)$ is an energetic parameter in Matsubara representation, Δ_n is a superconducting gap, μ^* is Coulomb pseudopotential, $\tilde{\Delta}$ is a renormalized gap and $\tilde{\varepsilon}_n$ is a renormalized energy parameter. The renormalization takes place due scattering of conduction electrons by impurities. Electron-phonon and electron-impurity coupling is represented by functions

$$L(n-m) = g \frac{\omega_{\text{D}}^2}{(n-m)^2 \pi^2 T^2 + \omega_{\text{D}}^2} \quad (23)$$

$$W(n-m) = \sum_A \sum_B \varpi_A \int_0^{2k_F} \int_0^\pi \frac{2\rho q dq \sin \theta d\theta}{\omega_{AB} v_F (2\pi)^2} |U(\mathbf{q}) \langle B|A \rangle_{\mathbf{q}}|^2 \frac{\omega_{AB}^2}{(n-m)^2 \pi^2 T^2 + \omega_{AB}^2}, \quad (24)$$

where v_F and k_F are Fermi velocity and Fermi momentum accordingly,

$$\langle B|A \rangle_{\mathbf{q}} = \int e^{-i\mathbf{q}\mathbf{r}} \phi_B^+ \phi_A d\mathbf{r}, \quad (25)$$

In a case of nonzero temperature $T \neq 0$ the impurities are distributed over states $|A\rangle, |B\rangle, |C\rangle, \dots$ with probability

$$\varpi_A = \frac{1}{Z} \exp\left(-\frac{E_A - E_0}{T}\right), \quad Z = \sum_A \exp\left(-\frac{E_A - E_0}{T}\right) \quad (26)$$

where E_0 is a ground state energy of an impurity, and the summation is extended on all possible states (we use a system of units where $\hbar = k_{\text{B}} = 1$). If impurities are harmonic oscillators then we can simplify Eq.(24):

$$W(n-m) \approx \int_0^{2k_F} \int_0^\pi \frac{2\rho q dq \sin \theta d\theta}{\omega_{AB} v_F (2\pi)^2} |U(\mathbf{q}) \langle B|A \rangle_{\mathbf{q}}|^2 \frac{\omega_{AB}^2}{(n-m)^2 \pi^2 T^2 + \omega_{AB}^2}, \quad (27)$$

where $|A\rangle$ is a ground state of the oscillator ($n=0, l=0, m=0$), $|B\rangle$ is the nearest excited state ($n=0, l=1, m=0$). Justification of the approximation (27) is given in Section III B in numerical calculations.

The gap $\tilde{\Delta}_m$ is an even function of $2m+1$, but the energy parameter $\tilde{\varepsilon}_m$ is an odd function of $2m+1$. Hence these functions are renormalized in different ways:

$$\frac{\tilde{\Delta}}{\tilde{\varepsilon}} > \frac{\Delta}{\varepsilon}. \quad (28)$$

This inequality ensures increasing of the gap Δ as compared with a pure superconductor or with a dirty superconductor with elastic impurities where an equality $\frac{\tilde{\Delta}}{\tilde{\varepsilon}} = \frac{\Delta}{\varepsilon}$ takes place. Thus Anderson theorem is violated in the sense that embedding of the impurities in s -wave superconductor increases its critical temperature.

The set of equations (19-22) can be simplified using an approximation for an electron-electron interaction amplitude $gw(\varepsilon_n, \varepsilon_{n'})$ with a method proposed in [27]:

$$w(\varepsilon_n, \varepsilon_m) \equiv \frac{\omega^2}{(\varepsilon_n - \varepsilon_m)^2 + \omega^2} \longrightarrow w(\varepsilon_n)w(\varepsilon_m) = \frac{\omega}{\sqrt{\varepsilon_n^2 + \omega^2}} \frac{\omega}{\sqrt{\varepsilon_m^2 + \omega^2}}. \quad (29)$$

Here $\omega = \omega_D, \omega_{AB}, \dots$ is characteristic frequency of the interaction. In addition we suppose the gap to be real $\Delta = \Delta^+$ and to depend on energy as follows:

$$\Delta_n = \Delta \frac{\omega_D}{\sqrt{\varepsilon_n^2 + \omega_D^2}} \equiv \Delta w_D(\varepsilon_n). \quad (30)$$

Moreover we can consider some effective electron-phonon coupling constant g instead of $g - \mu^*$ so that would have the correct critical temperature $T_C = 19.3\text{K}$ of a pure K_3C_{60} using the approximation (29). The approximation (29) removes contribution of terms with $m = n$ that is $L(0)$ and $W(0)$. The terms do not influence upon a gap and a critical temperature and they describe a scattering of electrons by thermal oscillations of the lattice and impurities [28]. The thermal oscillations behave like static impurities with effective concentration $\rho_{\omega_0}^{2T}$. The scattering gives an additional contribution in resistance of the metal analogously to a contribution of thermal phonons. Thus the terms with $m \neq n$ can violate Anderson's theorem only.

Then Eqs.(19-22) in the approximation (29) have a form

$$Z(\varepsilon_n)\Delta_n = g \sum_{m=-\infty}^{+\infty} \frac{\pi T \tilde{\Delta}_m}{\sqrt{\tilde{\varepsilon}_m^2 + |\tilde{\Delta}_m|^2}} w_D(\varepsilon_n) w_D(\varepsilon_m) \quad (31)$$

$$(1 - Z(\varepsilon_n))\varepsilon_n = g \sum_{m=-\infty}^{+\infty} \frac{\pi T \tilde{\varepsilon}_m}{\sqrt{\tilde{\varepsilon}_m^2 + |\tilde{\Delta}_m|^2}} w_D(\varepsilon_n) w_D(\varepsilon_m) = 0 \implies Z = 1, \quad (32)$$

$$\tilde{\Delta}_n = \Delta_n + G \sum_{m=-\infty}^{+\infty} \frac{\pi T \tilde{\Delta}_m}{\sqrt{\tilde{\varepsilon}_m^2 + |\tilde{\Delta}_m|^2}} w_{AB}(\varepsilon_n) w_{AB}(\varepsilon_m) \quad (33)$$

$$\tilde{\varepsilon}_n = \varepsilon_n + G \sum_{m=-\infty}^{+\infty} \frac{\pi T \tilde{\varepsilon}_m}{\sqrt{\tilde{\varepsilon}_m^2 + |\tilde{\Delta}_m|^2}} w_{AB}(\varepsilon_n) w_{AB}(\varepsilon_m) = \varepsilon_n + 0, \quad (34)$$

where G is electron-impurity coupling constant:

$$G = \int_0^{2k_F} \int_0^\pi \frac{2\rho q dq \sin \theta d\theta}{\omega_{AB} v_F (2\pi)^2} |U(\mathbf{q}) \langle B|A \rangle_{\mathbf{q}}|^2 \quad (35)$$

Then Eqs.(31-34) can be reduced to a form

$$\Delta = g \sum_{m=-\infty}^{+\infty} \frac{\pi T \tilde{\Delta}_m}{\sqrt{\tilde{\varepsilon}_m^2 + |\tilde{\Delta}_m|^2}} w_D(\varepsilon_m) \quad (36)$$

$$\tilde{\Delta}_m = \Delta w_D(\varepsilon_m) + \Delta w_{AB}(\varepsilon_m) \frac{f}{1 - h}, \quad (37)$$

where

$$f = G \sum_{n=-\infty}^{+\infty} \frac{1}{\sqrt{\pi^2 T^2 (2n+1)^2 + |\tilde{\Delta}_n|^2}} w_D(\varepsilon_n) w_{AB}(\varepsilon_n) \quad (38)$$

$$h = G \sum_{n=-\infty}^{+\infty} \frac{1}{\sqrt{\pi^2 T^2 (2n+1)^2 + |\tilde{\Delta}_n|^2}} w_{AB}^2(\varepsilon_n). \quad (39)$$

Our aim is to find critical temperature of the system. Then we have to suppose $\tilde{\Delta}(T_C) = \Delta(T_C) = 0$ in Eqs.(36,37). In this case Eq.(36) has form

$$\Rightarrow 1 = g^2 \sum_{n=-\infty}^{+\infty} \frac{1}{|2n+1|} \left[w_{\mathbf{D}}^2(\varepsilon_n) + w_{\mathbf{D}}(\varepsilon_n) w_{\omega_{AB}}(\varepsilon_n) \frac{G \Upsilon\left(\frac{\omega_{\mathbf{D}}}{\pi T}, \frac{\omega_{AB}}{\pi T}\right)}{1 - G \Xi\left(\frac{\omega_{AB}}{\pi T}\right)} \right], \quad (40)$$

where

$$\Upsilon\left(\frac{\omega_{\mathbf{D}}}{\pi T}, \frac{\omega_{AB}}{\pi T}\right) = \sum_{n=-\infty}^{+\infty} \frac{1}{|2n+1|} \frac{\omega_{\mathbf{D}}/\pi T}{\sqrt{|2n+1|^2 + (\omega_{\mathbf{D}}/\pi T)^2}} \frac{\omega_{AB}/\pi T}{\sqrt{|2n+1|^2 + (\omega_{AB}/\pi T)^2}} \quad (41)$$

$$\begin{aligned} \Xi\left(\frac{\omega_{AB}}{\pi T}\right) &= \frac{(\omega_{AB}/\pi T)^2}{|2n+1|^2 + (\omega_{AB}/\pi T)^2} \\ &= \left[\gamma + 2\ln 2 + \frac{1}{2} \Psi\left(\frac{1}{2} - \frac{i}{2} \frac{\omega_{AB}}{\pi T}\right) + \frac{1}{2} \Psi\left(\frac{1}{2} + \frac{i}{2} \frac{\omega_{AB}}{\pi T}\right) \right]. \end{aligned} \quad (42)$$

Here Ψ is a digamma function, $\gamma \approx 0.577$ is Euler constant. Transition temperature T_C^* of the system metal+impurity is temperature when equality (40) is satisfied. If the impurities are absent $G = 0$ we have an equation for critical temperature T_C of a pure metal:

$$\Rightarrow 1 = g^2 \sum_{n=-\infty}^{+\infty} \frac{1}{|2n+1|} w_{\mathbf{D}}^2(\varepsilon_n), \quad (43)$$

We can see that the right side of Eq.(40) has a singularity when

$$1 = G \Xi\left(\frac{\omega_{AB}}{\pi T}\right), \quad (44)$$

Temperature, when equality (44) is satisfied, is named *singularity temperature* T^* introduced in [4]. In terms of Eqs.(19-22) the singularity temperature is determined by homogeneous set of equations obtained from Eq.(24) omitting Δ_n :

$$\sum_m W(n-m) \frac{\tilde{\Delta}_m}{|\varepsilon_m|} - \tilde{\Delta}_n = 0 \quad (45)$$

A determinant of the set of equations (45) must be equal to zero:

$$\det D_{mn}(T_C^*) = 0, \quad D_{mn} = \frac{W(n-m)}{|\varepsilon_m|} - \delta_{mn}, \quad (46)$$

where $\delta_{mn} = 1$ if $m = n$, $\delta_{mn} = 0$ if $m \neq n$. If an interaction with impurities is nonretarded (elastic): $W(n-m) = W(0)\delta_{mn}$, then the singularity temperature is absent [5]. Thus Anderson theorem is realized for the elastic interaction: $T_C^* = T_C$. The singularity temperature is $T^* < T_C^*$ and it can be used as a lower estimation of the critical temperature of the system. Its physical sense is: the singularity temperature is a superconducting transition temperature if we turn off the pairing interaction caused by metal's phonon.

Eq.(44) is simpler than Eq.(46). Limit cases of Eq.(44) are

$$\begin{aligned} \Xi\left(\frac{\omega_{AB}}{T} \rightarrow 0\right) &\rightarrow \frac{7}{4} \zeta(3) \left(\frac{\omega_{AB}}{\pi T}\right)^2 \Rightarrow T^* = \frac{\sqrt{7\zeta(3)}}{2\pi} \omega_{AB} \sqrt{G} \\ \Xi\left(\frac{\omega_{AB}}{T} \rightarrow \infty\right) &\rightarrow \ln\left(\frac{2}{\gamma} \frac{\omega_{AB}}{\pi T}\right) \Rightarrow T^* = \frac{2\omega_{AB}}{\pi\gamma} \exp\left(-\frac{1}{G}\right). \end{aligned} \quad (47)$$

Thus the limit cases (47) correspond to limit cases for critical temperature of a metal superconductor in Eliashberg equations [29].

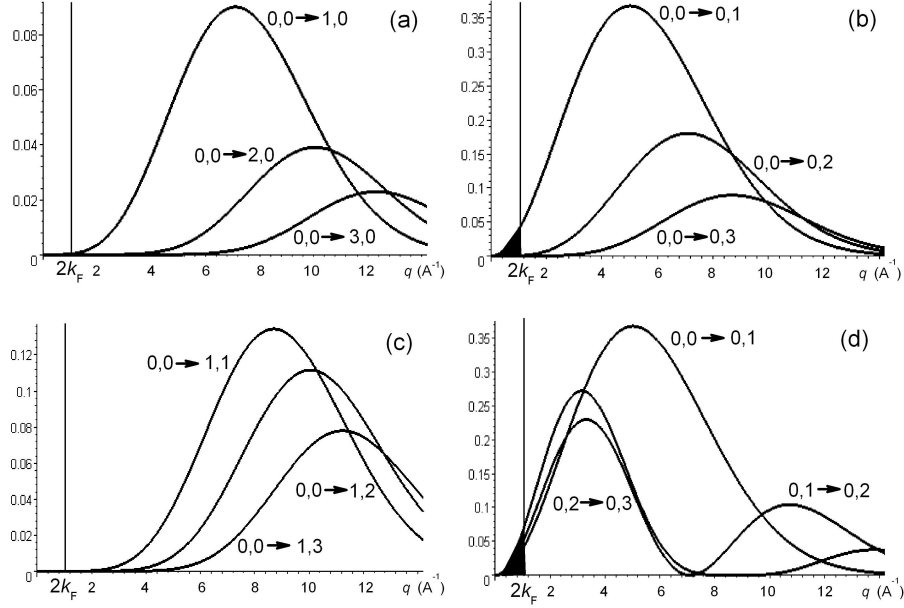


Рис. 3: Amplitudes $\langle B|A \rangle_{\mathbf{q}}$ (25) for transitions $n, l \rightarrow n', l'$ of 3D harmonic oscillator. Interval $(0, 2k_F)$ of integration in Eq.(24) is painted over.

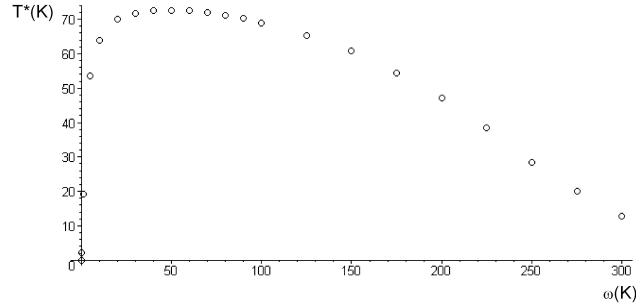


Рис. 4: Dependence of the singularity temperature T^* of $K_3\text{He}@C_{60}$ on the oscillation frequency of a helium atom in an endohedral fullerene.

B. Calculation of the singularity temperature and the transition temperature.

In this section we calculate the singularity temperature and the transition temperature for $K_3\text{He}@C_{60}$ using Eqs.(15,35,40,44). Data for K_3C_{60} are given from [30]. First, let us consider the transition amplitude $\langle B|A \rangle_{\mathbf{q}}$ (25) for various states $|A\rangle$ and $|B\rangle$ of 3D harmonic oscillator. State of the oscillator is determined with three quantum numbers n, l, m . Energy of the oscillator is (5). Ground state is $0, 0, 0$. A value (25) is not equal to zero only for transition when $\Delta m = 0$. Results of the calculation for some transitions are shown in Fig.3. In Eq.(24) we integrate over momentum from zero to $2k_F = 0.92\text{\AA}^{-1}$. This interval is painted over in Fig.3. We can see transitions with $\Delta n = 0, \Delta l = \pm 1$ give contribution in the integral (24) only, moreover the contributions of transitions $l \rightarrow l \pm 1$ are approximately equal for arbitrary orbital quantum number l . For the harmonic oscillator spectrum (5) energy of the transitions $l \rightarrow l \pm 1$ are equal $\Delta E(\Delta n = 0, \Delta l = \pm 1, \Delta m = 0) = \omega$. Thus the approximation (27) can be used where a state $|A\rangle = \Psi_{0,0,0}(r, \theta, \varphi)$ is a ground state and a state $|B\rangle = \Psi_{0,1,0}(r, \theta, \varphi)$ is the first excited state with

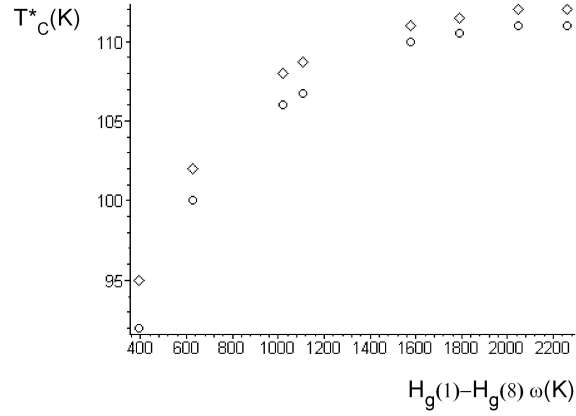


Рис. 5: The critical temperature T^* of $K_3He@C_{60}$ for each oscillation frequency of intramolecular modes $H_g(1) - H_g(8)$ of an fullerene (if only one frequency takes a role in pairing of electron and all the rest frequencies do not play a part in this process). Circle symbols - for the frequency of a helium atom in an endohedral fullerene $\omega_1 = 151K$, diamond symbols for the frequency $\omega_1 = 128K$.

$n = 0, l = 1, m = 0$, because

$$\begin{aligned} & \int_0^{2k_F} \int_0^\pi \frac{2\rho q dq \sin \theta d\theta}{\omega v_F (2\pi)^2} |U(\mathbf{q}) \langle \Psi_{0,1,0} | \Psi_{0,0,0} \rangle \mathbf{q}|^2 \frac{\omega^2}{(n-m)^2 \pi^2 T^2 + \omega^2} \\ & \approx \int_0^{2k_F} \int_0^\pi \frac{2\rho q dq \sin \theta d\theta}{\omega v_F (2\pi)^2} |U(\mathbf{q}) \langle \Psi_{n,l\pm 1,m} | \Psi_{n,l,m} \rangle \mathbf{q}|^2 \frac{\omega^2}{(n-m)^2 \pi^2 T^2 + \omega^2}, \\ & \sum_A \varpi_A = 1 \end{aligned} \quad (48)$$

Let us calculate the singularity temperature T^* using Eqs.(35,44). In a potential $U(q)$ (15) we can suppose $E = E_{4s} = -4.44eV$ - energy of a valent state of kalium. Dependence of the temperature T^* on oscillation frequency of a helium atom in an endohedral fullerene is shown in Fig.(4). We can see the dependence $T^*(\omega)$ seems to an effectiveness function in [4]. For frequencies (3,4) from model [19] we have results:

$$\omega_1 = 151K, \quad T^* = 60.4K \quad (49)$$

$$\omega_2 = 128K, \quad T^* = 65.1K. \quad (50)$$

Let us calculate the critical temperature T_C^* . Conduction electrons interact with intramolecular $H_g(1) - H_g(8)$ phonons, which have frequencies $391 \div 2257K$ [25]. Each vibrational mode is characterized by own coupling constant with electrons. Interaction with the intramolecular phonons results to superconductivity of alkali-doped fullerenes. In order to calculate the critical temperature we propose a following method. We know that critical temperature of K_3C_{60} is $T_C = 19.3K$. We can assume that this critical temperature can be obtained with each vibrational mode of fullerene separately - when only one frequency takes a role in pairing of electron and all the rest frequencies do not play a part in this process. Corresponding coupling constants g can be calculated by a formula:

$$\Rightarrow 1 = g \sum_{n=-\infty}^{+\infty} \frac{1}{|2n+1|} w_{\omega_D}^2(\varepsilon_n), \quad (51)$$

then we have

| | $H_g(1)$ | $H_g(2)$ | $H_g(3)$ | $H_g(4)$ | $H_g(5)$ | $H_g(6)$ | $H_g(7)$ | $H_g(8)$ |
|---|----------|----------|----------|----------|----------|----------|----------|----------|
| | 391K | 626K | 1018K | 1110K | 1575K | 1792K | 2047K | 2257K |
| g | 0.320 | 0.280 | 0.250 | 0.240 | 0.225 | 0.22 | 0.21 | 0.205 |

(52)

Then with help of Eqs.(35,40) we can calculate T_C^* of $K_3He@C_{60}$. Results for two frequencies (49,50) are shown in Fig.(5). We can see that the critical temperature is within the interval $T_C^* = 92 \div 112K$, that is it varies little while the frequencies $H_g(1) - H_g(8)$ vary essentially $391 \div 2257K$, thus our method is correct.

IV. CONCLUSION.

In this paper we have proposed the model of an impurity with retarded interaction with quasiparticle. As an impurity we suggest to use endohedral complexes - a helium atom inside C_{60} cage: $He@C_{60}$. The atom in the carbon cage is a oscillator with frequency $\sim 150K$, where we assume that oscillations of the central atom and carbon cage are independent. Endohedral fullerenes with a noble atom inside (He , Ne , Ar , Kr , Xe) has symmetry and chemical properties as the hollow fullerenes. We propose to use an alkali-doped fullerenes (K_3C_{60} , Rb_3C_{60} etc.) as a conducting matrices where these impurity can be applied. These matrices allow us to create a large concentration of impurities $\rho = 4/a$ (where a is a lattice constant) without reduction in the density of states on Fermi surface. Thus we considered a new hypothetical substance $K_3He@C_{60}$, where the helium atom can be considered as impurities, because the averaging over disorder (17) and the jelly model lead to the same result - mean-field effect on the conduction electrons. We have shown potential of interaction of the impurities with electrons is a pseudopotential (7) which can be localized to a potential (15). Based on results of works [4, 5] we have calculated singularity temperature which is introduced in these works and it is important characteristic of a system matrix+impurity, and we have calculated critical temperature of the system $K_3He@C_{60}$. The singularity temperature is within the limits $60.4 \div 65.1K$ - Fig.(4) and the critical temperature is within the limits $92 \div 112K$ - Fig.(5). Thus effect of the impurities on critical temperature of alkali-doped fullerene is very strong. However, it should be noted the pseudopotential is ambiguous [21], and it must have fitting parameters. Hence the obtained results must be considered as evaluation only.

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